

A “Gaussian” for diffusion on the sphere

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Abstract –We present an analytical closed form expression, which gives a good approximate propagator for diffusion on the sphere. Our formula is the spherical counterpart of the Gaussian propagator for diffusion on the plane. While the analytical formula is derived using saddle point methods for short times, it works well even for intermediate times. Our formula goes beyond conventional “short time heat kernel expansions” in that it is nonperturbative in the spatial coordinate, a feature that is ideal for studying large deviations. Our work suggests a new and efficient algorithm for numerical integration of the diffusion equation on a sphere. We perform Monte Carlo simulations to compare the numerical efficiency of the new algorithm with the older Gaussian one.

Introduction: Diffusion on the sphere is a problem that arises in several contexts. At the cellular level, diffusion is an important mode of transport of substances. The cell wall is a lipid membrane and biological substances like lipids and proteins diffuse on it. In general biological membranes are curved surfaces. Spherical diffusion also crops up in the swimming of bacteria, surface smoothening in computer graphics [1] and global migration patterns of marine mammals [2]. Such diffusion effects are studied using computer simulations. There have been experimental studies of fluorescent marker molecules on curved surfaces like micelles and vesicles [3, 4] using fluorescence anisotropy decay.

While diffusion in Euclidean space has been studied extensively both analytically and numerically [5, 6], there have been fewer studies of diffusion on curved surfaces. There have been some analytical studies of diffusion on curved surfaces [7–9]. Some of these studies [7, 8] arrive at a short time heat kernel expansion [10–12] for the probability distribution. This expansion is perturbative in the time step as well as the spatial step as is evident from Eq. (51) of Ref. [8]. However, there does not exist a simple closed form analytical expression, for the probability distribution for diffusion on a curved surface which can be implemented in a computer simulation. Here we focus on diffusion on a sphere, the case of a curved surface

with constant positive curvature. The simplest and most natural method of generating diffusion on a curved manifold is to consider a large number of walkers performing a random motion. The random walkers can be described by a Langevin equation using a spatial step size much smaller than the inverse curvature so that curvature can be neglected. In this “tangent space” approximation, the sphere appears locally flat and one can ignore its curvature. This is the approach taken for example in [3, 4] in which the diffusing particle takes a Brownian step in the tangent plane at a point on S^2 and is then projected back to the surface of the sphere. One can describe the ensemble of random walkers with a probability distribution P and write a Fokker-Planck (diffusion) equation governing the spread of probability. One finds (see page 847 of Ref. [13]) on general grounds, the temporal step size must be chosen smaller than the square of the spatial step size. As a result of the small spatial step size forced on us by the tangent space method, integrating in time is computationally expensive. It would be useful to have a method which permits larger step sizes, not constrained by the curvature.

There has been some work [14, 15] generating an algorithm for diffusion on S^2 by making use of known analytic results on S^3 , the hypersphere in four dimensions and identifying S^2 with a thin strip around the equator of S^3 with a reflecting boundary. These methods give

rise to an improved algorithm for treating diffusion on S^2 . However, the use of S^3 and the method of dimensional reduction render the treatment less than intuitive. Our purpose here is to provide a more down to earth approach by working *directly* on S^2 . We derive an approximate analytical formula for the distribution function representing diffusion on a sphere. In contrast to earlier studies [7, 8] we use a semiclassical saddle point approximation which is perturbative in time but *nonperturbative in space*. Our formula reduces to the formula presented in [7, 8] in the limit of small spatial scales. In the planar limit our formula reduces to a Gaussian. We use our “Gaussian” on the sphere to generate an efficient algorithm for simulating Brownian motion on a sphere. The algorithm improves over the earlier tangent space simulation algorithm. We expect this algorithm to have a wide range of applications, especially in fields where one needs to repeatedly generate diffusion processes on spheres. In the physics of stiff, inextensible polymers, one has constraints on the bond lengths while the bond angles are relatively unconstrained. This leads to random motions, as in the Kratky-Porod model which represent diffusion on spheres. In computer graphics, one seeks algorithms which can be used to smooth graphical data on spherical images. A standard technique is to use the diffusion equation on the sphere, but a simple and accurate algorithm for implementing this is presently lacking.

Theory: To define our problem regarding diffusion on a sphere, consider first diffusion on a plane which is described by

$$\frac{\partial P}{\partial t}(\vec{x}, t) = D \nabla^2 P(\vec{x}, t) \quad (1)$$

where D is the diffusion constant and $P(\vec{x}, t)$ the probability distribution on the plane at time t . The elementary solution with initial distribution $P(\vec{x}, 0) = \delta^2(\vec{x})$ is easily found by Fourier transform. The formal solution is

$$P(\vec{x}, t) = \frac{1}{4\pi^2} \int d\vec{k} e^{-D\vec{k} \cdot \vec{k}t} e^{i\vec{k} \cdot \vec{x}} \quad (2)$$

which can be integrated to give a simple Gaussian form

$$P(\vec{x}, t) = \left(\frac{1}{4\pi Dt} \right) \exp -\frac{\vec{x} \cdot \vec{x}}{4Dt} \quad (3)$$

When expressed in plane polar co-ordinates (r, θ) , the probability distribution function in r is

$$P(r, t) = \left(\frac{r}{2Dt} \right) \exp -\frac{r^2}{4Dt} \quad (4)$$

While these two expressions (2,4) are formally equal to each other, the first is an unwieldy integral whereas the second is a simple closed form Gaussian expression which is well suited to numerical work. In (2) the time t appears in the numerator of the exponent leading to slow convergence for small times, unlike (4) where it appears in the denominator. Our purpose in this Letter is to seek the analogue of (4) for spherical diffusion.

Consider the analogous situation on the sphere

$$S^2 = \{(x^1, x^2, x^3) \in \mathbb{R}^3 : (x^1)^2 + (x^2)^2 + (x^3)^2 = R^2\} \quad (5)$$

of radius R in three dimensional Euclidean space. In standard polar coordinates on the sphere the diffusion equation is

$$\frac{\partial P}{\partial t} = \frac{D}{R^2} \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial P}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 P}{\partial \varphi^2} \right) \quad (6)$$

Let us define a dimensionless time variable $\tau = 2Dt/R^2$ for convenience. Typical values for diffusion on a lipid membrane are $R = 1\mu\text{m}$ and $D = 1\mu\text{m}^2/\text{sec}$. The τ values of interest to us are on the order of seconds.

For an initial θ distribution $P(\theta, 0)$ (including the measure $\sin \theta$) with δ function support at the North pole $\theta = 0$, the diffusion equation has a formal solution for the final distribution in θ at time τ :

$$P(\theta, \tau) = \frac{\sin \theta}{2} \sum_{l=0}^{\infty} (2l+1) e^{-l(l+1)\tau/2} P_l(\cos \theta). \quad (7)$$

Such a solution is formally exact and analogous to (2), but in practice, unwieldy to use in numerical work since it is expressed as an infinite series. For short times, the convergence of the series is poor and truncation leads to spurious oscillations.

Is there an analogue of the Gaussian form (4) on the sphere? The main result of this Letter is a closed form approximate expression which generalises the planar Gaussian (4) to the sphere. This approximate expression is given by:

$$Q(\theta, \tau) = \frac{\mathcal{N}(\tau)}{\tau} \sqrt{\theta \sin \theta} e^{-\frac{\theta^2}{2\tau}} \quad (8)$$

where $\mathcal{N}(\tau)$ is a constant determined by the normalisation condition

$$\int_0^\pi d\theta Q(\theta, \tau) = 1 \quad (9)$$

In the limit of small times, the expression (8) reduces to $\frac{1}{\tau} \exp -\frac{\theta^2}{2\tau}$ which agrees with the planar Gaussian (4). Our study shows that this expression turns out to be a good approximation to the exact propagator (7) even for intermediate times.

The Heat Kernel Expansion (HKE) results in a propagator (see Eq. 51 in Ref. [8]) expressed as a power series in θ

$$Q_{HKE}(\theta, \tau) = \frac{1}{\tau} \left(1 + \frac{\theta^2}{12} + \dots \right) e^{-\frac{\theta^2}{2\tau}} \sin \theta \quad (10)$$

where we have transcribed the content of Eq. 51 in Ref. [8] (suitably restricted to constant curvature) and inserted the measure factor of $\sin \theta$ for easy comparison. The new propagator is essentially a summation of this perturbative series.

Figures 1 and 2 show a comparison of the exact propagator (with the upper limit l_{max} in the summation set to 20) with the approximate one for a range of τ . The

plots of Fig. (1) show $P(\theta, \tau)$ and $Q(\theta, \tau)$ for $\tau = .5, 1$ and $Q(\theta, \tau)_{HKE}$ truncated to the second term.

The deviation between probability distributions can be quantitatively measured using the Kullback-Leibler divergence, which is also known as the relative entropy. This measure which is widely used in information theory [16] gives a positive number D_{KL} which measures the extent of deviation (or divergence) between a trial distribution $Q(\theta)$ and a fiducial one $P(\theta)$:

$$D_{KL} := \int_0^\pi d\theta P(\theta) \log \left[\frac{P(\theta)}{Q(\theta)} \right] \quad (11)$$

D_{KL} vanishes if and only if the two normalised distributions are identical. D_{KL} is also invariant under changes of coordinates. For the fiducial distribution we use the exact form (7) and compare KL divergence of the Gaussian propagator (restricted to the interval $[0, \pi]$ and normalised in this interval), the Q_{HKE} (10) as well as our new distribution Q_{new} . The table shows a comparison of D_{KL} Gaussian, D_{KL} HKE and D_{KL} new, for different values of τ .

Note that the new propagator always has a smaller KL divergence than the Gaussian propagator and Q_{HKE} . It is thus a better approximation to the exact propagator.

time τ	D_{KL} Gaussian	D_{KL} HKE	D_{KL} new
0.1	1.4×10^{-4}	6.5×10^{-7}	1.8×10^{-9}
0.5	4.0×10^{-3}	3.7×10^{-4}	3.8×10^{-6}
0.7	8.2×10^{-3}	1.3×10^{-3}	2.9×10^{-5}
0.9	1.3×10^{-2}	2.9×10^{-3}	9.9×10^{-5}
1.0	1.6×10^{-2}	3.9×10^{-3}	1.6×10^{-4}
2.0	4.3×10^{-2}	1.1×10^{-2}	8.9×10^{-4}

Derivation of the Main Result: The elementary solution to the diffusion equation on the unit sphere is given by the Wiener integral [17]

$$K(\hat{n}_1, 0, \hat{n}_2, \tau) = \int \mathcal{D}[\hat{n}(\tau)] \exp -S[\hat{n}(\tau)] \quad (12)$$

where

$$S[\hat{n}(\tau)] = \frac{1}{2} \int_0^\tau \frac{d\hat{n}}{d\tau} \cdot \frac{d\hat{n}}{d\tau} d\tau. \quad (13)$$

$K(\hat{n}_1, 0, \hat{n}_2, \tau)$ is the conditional probability that the particle will be at \hat{n}_2 at time τ given that it was at \hat{n}_1 at time 0. For short times τ , we may use a semiclassical approximation [18]

$$K(\hat{n}_1, 0, \hat{n}_2, \tau) = \mathcal{N}(\tau) \sqrt{\det V} \exp -S_{cl}[\hat{n}_1, \hat{n}_2, \tau] \quad (14)$$

where $S_{cl}[\hat{n}_1, \hat{n}_2, \tau]$ is defined as the classical action of the least action path connecting \hat{n}_1 to \hat{n}_2 in “time” τ . The least action path is unique if \hat{n}_1, \hat{n}_2 are not collinear, which we assume and thus exclude the isolated points $\theta = 0, \pi$. $\det V$ is the Van Vleck determinant given by the determinant of the 2×2 Hessian matrix

$$V_{ij} = \frac{\partial^2 S_{cl}[\hat{n}_1, \hat{n}_2, \tau]}{\partial \hat{n}_1^i \partial \hat{n}_2^j} \quad (15)$$

and \mathcal{N} is a normalisation constant.

Varying the action to find the classical path yields the geodesic equation

$$\frac{d^2 \hat{n}}{d\tau^2} = \lambda \hat{n}, \quad (16)$$

where λ is a Lagrange multiplier enforcing the constraint $\hat{n} \cdot \hat{n} = 1$. The solution to (16) is the unique great circle passing through \hat{n}_1 and \hat{n}_2 . The classical action is given by

$$S_{cl} = \theta^2 / 2\tau \quad (17)$$

where $\cos \theta = \hat{n}_1 \cdot \hat{n}_2$ defines θ , $0 < \theta < \pi$, the length of the shortest geodesic arc connecting \hat{n}_1 to \hat{n}_2 . From an evaluation of the Van Vleck determinant

$$\det V = \hat{n}_{1p} \epsilon^{pil} \hat{n}_{2q} \epsilon^{qjk} V_{ij} V_{lk}$$

we find that

$$\det V = \frac{\theta}{\tau^2 \sin \theta}. \quad (18)$$

This leads to the approximate propagator

$$K[\hat{n}_1, 0, \hat{n}_2, \tau] = \frac{\mathcal{N}(\tau)}{\tau} \sqrt{\theta / \sin \theta} e^{-\frac{\theta^2}{2\tau}}. \quad (19)$$

Multiplying by the measure $\sin \theta$ to convert into a θ distribution leads to the approximate propagator which is used in eq.(8).

Computer Simulations: We have performed Monte Carlo simulations of spherical diffusion to investigate the numerical efficacy of the approximate propagator derived analytically in the last section. The Fokker-Planck equation on a sphere is exactly solvable and the solution can be expressed as a series involving the Legendre polynomials as described earlier. However, because of poor convergence of the series for short times, this form is not suitable for repeated numerical evaluation. We use the exact solution with a comfortably large cutoff $l_{max} = 20$ as a standard against which the computer simulations are tested.

In performing the simulations, we have closely followed the method adopted in Ref. [3, 4] for studying diffusion of fluorescent molecules on a sphere. We have studied the diffusion of 5×10^6 molecules and obtained the distribution of the final polar angular displacement θ .

To integrate for a time τ , we split up the time interval τ into n_{step} time steps $\tau = n_{step} \tau_{step}$ each of size τ_{step} . The value of τ_{step} determines the spatial step size σ via the standard diffusion relation

$$\tau_{step} = \frac{\sigma^2}{2} \quad (20)$$

We have implemented two distinct algorithms for randomly choosing β : a Gaussian algorithm and our proposed new algorithm. In the first algorithm, we replace the spherical geometry locally by the tangent plane to the sphere at the starting point of each Monte Carlo move. Confining ourselves to the local tangent plane on

the sphere at each move, we choose β according to the distribution (eq. 4)

$$Q_{Gauss}(\beta) = \frac{2\beta}{\sigma^2} \exp(-\beta^2/\sigma^2). \quad (21)$$

Thus at each step, the angular displacement β is chosen from a two dimensional Gaussian distribution which has zero mean and standard deviation σ . This is our first algorithm. It is only expected to be accurate when the step size σ is small.

In the second method, the angular displacement at each step was chosen from the approximate propagator given by (8).

$$Q_{new}(\beta) = \frac{2\mathcal{N}}{\sigma^2} \sqrt{\beta \sin \beta} \exp(-\beta^2/\sigma^2) \quad (22)$$

This distribution reduces to the previous one (21) when the step size σ is small, but has a larger range of validity since it takes into account the curvature of the sphere.

In both algorithms the random numbers were generated by constructing a random walk of the variable β in the external potential $-\log Q(\beta)$. After discarding 10^5 steps to get rid of transients, we arrange the subsequent 10^6 β values as a $10^3 \times 10^3$ matrix, transpose it and store the values for use in the program. This shuffles the random numbers and removes correlations between neighboring steps.

Whereas the planar Gaussian algorithm needs to use small displacements to ensure that the tangent plane approximation remains valid, the proposed new algorithm is not constrained by this requirement. It remains a good approximation even for intermediate σ . As a result in order to integrate for $\tau = 2$, we need to use just two time steps with a step size of $\sigma = 1.414$ with the new algorithm (Figure 3). With the Gaussian algorithm, even with eight time steps of step size $\sigma = .7071$, one achieves a poorer accuracy (Figure 4). This new algorithm is our second main point in this Letter.

Conclusion. — In this Letter we derive an approximate analytical formula for the distribution function for spherical diffusion and use it to generate a simple and efficient algorithm for simulations. While we have restricted ourselves to spherical diffusion, it is evident that our results apply equally well to the saddle, (or hyperbolic plane), the space of constant negative curvature. The only change is that the circular function $\sin \theta$ is replaced by the hyperbolic function $\sinh \theta$. Our results for the approximate propagator (19) also extend to higher (D) dimensional spheres and saddles with the slight modification that the prefactor $\theta/\sin \theta$ (or its hyperbolic form) is replaced by $(\theta/\sinh \theta)^{\frac{D-1}{2}}$.

Rasin et al [19] studied diffusion on a planar lattice and addressed the problem of scaling of the time step as the square of the lattice size. Their solution uses kinetic methods that replace the parabolic diffusion equation by a hyperbolic one, thus allowing for larger time evolution steps. It would be interesting to extend their work, using

a variable coordination number on the lattice to encode curvature [20].

For a general curved surface embedded in three dimensional space, the intrinsic geometry is determined entirely by the Gaussian curvature κ . Since diffusion on the surface depends *only* on the intrinsic geometry, we may consider each part of the surface as locally approximated by a sphere of radius $R = 1/\sqrt{\kappa}$. We may then apply the new simulation algorithm described in this paper in a local patch. This entails numerically introducing geodesic based coordinates and choosing isotropically distributed steps, with a size distribution given by (22). We expect this to improve on the tangent space simulation methods, since these only approximate the local geometry to first order and do not take into account the second order effects of curvature. The new propagator would be useful in a wide variety of applications.

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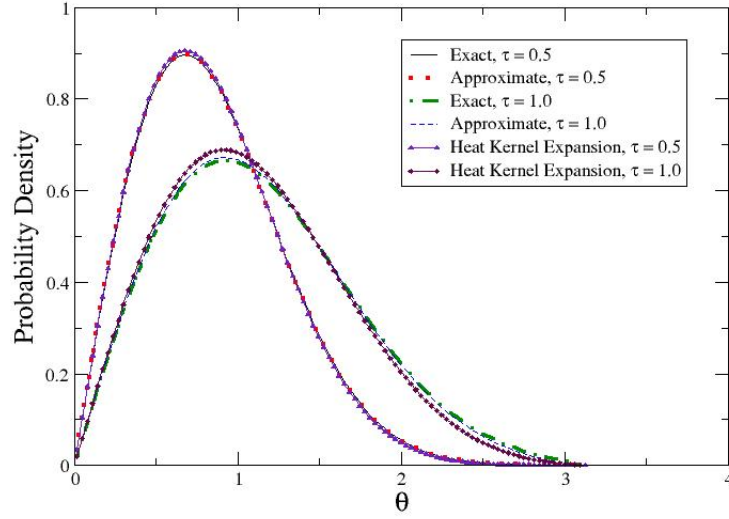


Fig. 1: (Colour online) Figure shows a comparison of the exact propagator (Eq. (7) truncated to $l_{max} = 20$), the approximate one Eq. (8) and the Heat Kernel expansion for $\tau = 0.5, 1.0$. Note that the difference between the first two is barely discernible.

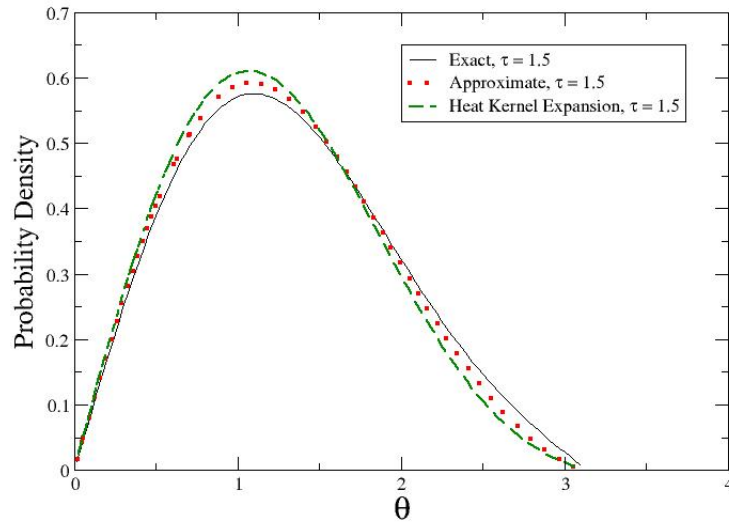


Fig. 2: (Colour online) Figure shows a comparison of the exact propagator (Eq. (7) truncated to $l_{max} = 20$) with the approximate one (Eq. (8)) for $\tau = 1.5$. The difference is now apparent. Also shown is the Heat Kernel expansion, which differs even more from the exact propagator.

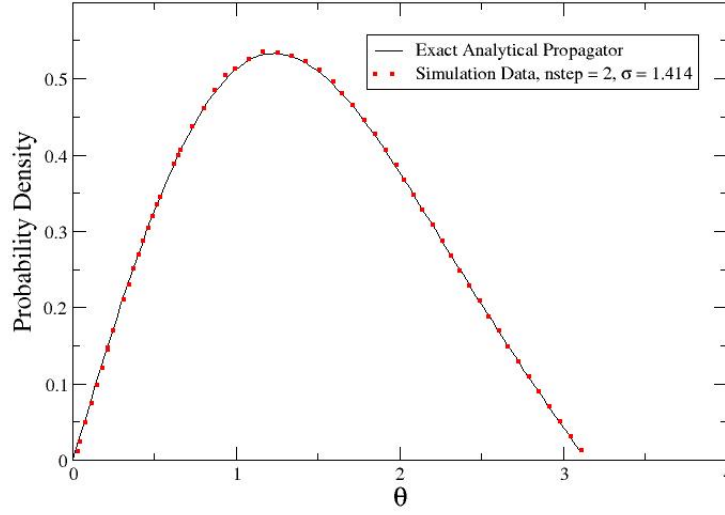


Fig. 3: (Colour online) Figure shows a comparison of the exact propagator with the simulation data using the new algorithm. The total time τ of integration is $\tau = 2$ and this time has been achieved with two steps, each of step size $\sigma = 1.414$.

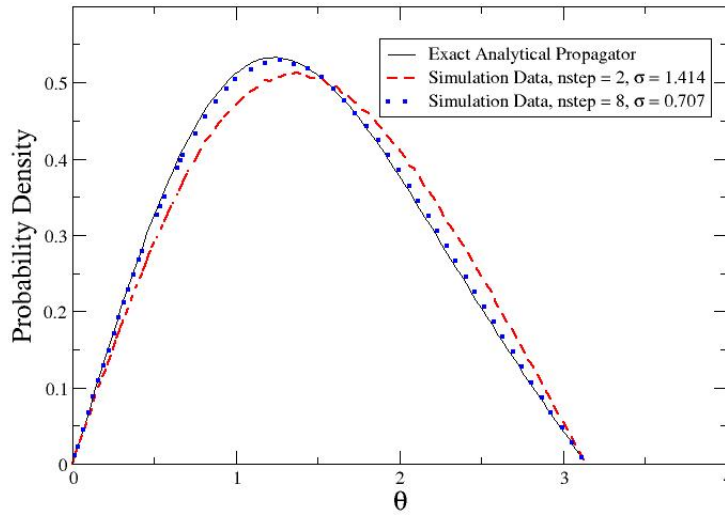


Fig. 4: (Colour online) Figure shows a comparison of the exact propagator with the simulation data using the Gaussian algorithm. The total time τ of integration is $\tau = 2$ and this time has been achieved with two steps of step size $\sigma = 1.414$ (dashed curve) and eight steps of size $\sigma = .7071$. Notice that the Gaussian algorithm requires a larger number of steps to reproduce the exact analytical propagator.